Project Status Report

High End Computing Capability
Strategic Capabilities Assets Program

April 10, 2015

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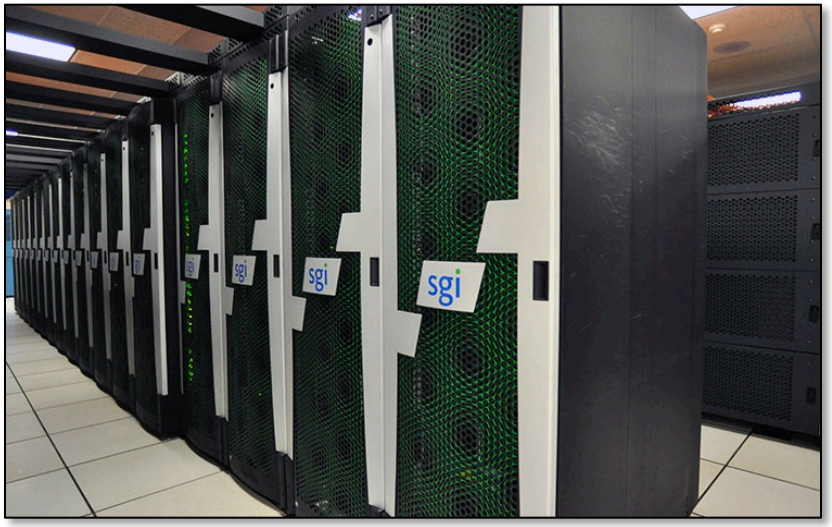
Pleiades Augmented with NVIDIA K40 Graphics Processing Units

- HECC engineers upgraded the Pleiades supercomputer with 64 Sandy Bridge nodes equipped with NVIDIA Tesla K40 graphics processing units (GPUs).
- Each of these nodes contain 64 gigabytes (GB) of memory, with each Tesla K40 GPU having a separate 12 GB of memory.
- HECC engineers worked with users to evaluate several hardware configurations for the Tesla K40 GPUs within the nodes to identify the optimal configuration.
- These additional GPU nodes, procured in collaboration with LaRC, augment 64 Westmere nodes containing NVIDIA Tesla M2090 GPUs that have been available on Pleiades since 2011.
- User support and documentation staff made significant changes to the HECC Knowledge Base article, "GPU Basics," and updated 5 related articles to help users quickly take advantage of the GPU technology.

Mission Impact: The addition of graphics processing units enables HECC users to utilize new technology to accelerate their demanding science and engineering applications running on HECC resources.



The Pleiades supercomputer was upgraded with 64 Sandy Bridge nodes repurposed from a testbed system and equipped with graphics processing units.

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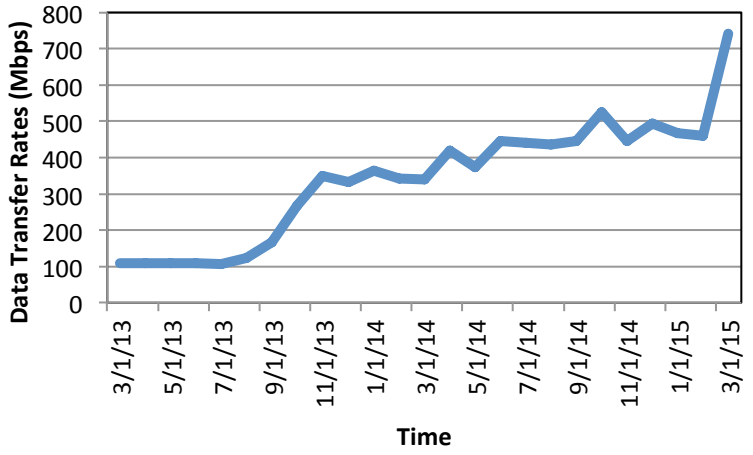
HECC Experts Team Up with JPL to Engineer Improvements in Network Performance

- Since March 2013, ongoing issues with security firewalls, over-saturated network paths, and switch buffers at Jet Propulsion Laboratory (JPL) caused greatly reduced file transfer rates for HECC users.
- Engineers on the HECC Networks team collaborated with JPL on system and application tuning and network buffering, and worked with NASA wide area network engineers to help reduce network saturation issues at JPL.
- The HECC team obtained accounts on JPL systems, isolated and proved the problems, completed troubleshooting, and tested transfer rate performance from both ends of the network.
- The team used in-house and standard, commercial off-the-shelf software tools to perform this work, and achieved a 750% improvement in network performance between the NASA Advanced Supercomputing (NAS) facility and JPL.
- HECC users at JPL frequently transfer very large datasets to and from the NAS facility for their mission research. Increasing the data transfer rates allows these users to quickly analyze their datasets and retrieve their data.

Mission Impact: Increasing data transfer rates for very large (multiple-terabyte) datasets vastly decreases time-to-solution, sometimes saving NASA scientists valuable hours or days of waiting to analyze and/or retrieve their data.



This graph shows the observed data transfer rate in megabits per second (Mbps) from March 2013 to today. The blue line indicates the average network performance.

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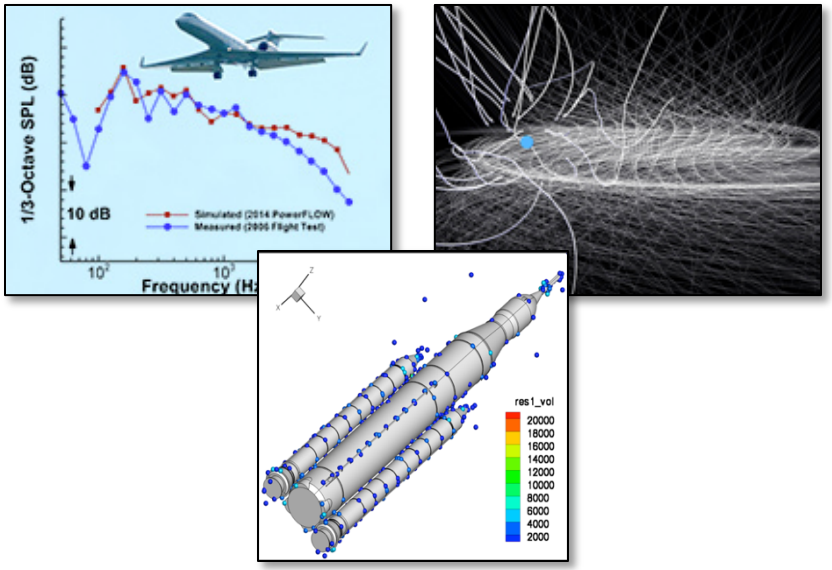
March 2015 Usage on Pleiades Sets New Monthly Record of 16.57 Million SBUs

- March usage on the Pleiades supercomputer set a new monthly record.
- Over 16.57 million Standard Billing Units (SBUs*) were used by NASA's science and engineering organizations, surpassing the previous record of 14.09 million SBUs (set in December 2014) by over 17%.
- This increase was enabled by high demand, system stability, and efficient operations that delivered over 85% system utilization (75% utilization is the target).
- Over 330 projects from all across NASA used time on Pleiades during March.
- Usage for the top 10 projects ranged between 384,214 and 1,410,032 SBUs, and accounted for over 43% of total usage.
- The HECC Project continues to plan and evaluate ways to address the future requirements of NASA's users.

*1 SBU equals 1 hour of a Pleiades Westmere 12-core node.

Mission Impact: Increasing Pleiades' system capacity provides Mission Directorates with more resources for the accomplishment of their goals and objectives.



Images from projects that were among the top users in their respective mission directorates. Clockwise from top left: Comparison between measured and simulated far-field noise spectra for a full-scale Gulfstream aircraft during landing. *Mehdi Khorrami, NASA/Langley.* Visualization of the JF12 coherent field model with 3D ultra-high-energy cosmic ray trajectories. *Michael Sutherland, Ohio State University; Glennys Farrar, New York University.* Computation of the transonic flow about a Space Launch System configuration. *Stephen Alter, NASA/Langley.*

POC: Catherine Schulbach, catherine.h.schulbach@nasa.gov, (650) 604-3180, NASA Advanced Supercomputing Division

Changes to Usage Accounting Improve Support for Dual Allocation Periods for SMD

- The HECC program's infrastructure for managing allocations of computer time was improved by automating the ability to support multiple allocation periods and allocation periods that do not begin on May 1.
- This is especially important for the Science Mission Directorate (SMD), which has two allocation periods per year, and for the Aeronautics Research Mission Directorate, which begins allocations on November 1 each year.
- Previously, processing for allocation periods that did not begin May 1 each year was done manually, and usage and allocations were not always clear to SMD users.
- Modifications that were done include: setting the allocation year to better match the calendar year, including a start date for allocations; and updating the job accounting utilities to display data based on the start date of the allocations instead of May 1.

Mission Impact: Automating and improving accounting processes provides better support to users, reduces user confusion, and lowers the risk of errors compared to manual processes.

Project	Host/Group	Fiscal Year	Used	% Used	Limit	Remain	Linear YTD Usage	Project Exp Date
g26113	pleiades	2014	82033.628	45.58	179993.000	97959.372	50.58	04/30/15
g26119	pleiades	2014	0.000	0.00	8533.000	8533.000	0.00	04/30/15
g26120	pleiades	2014	133901.834	55.11	242991.000	109089.166	61.15	04/30/15
g26122	pleiades	2014	0.000	0.00	13860.000	13860.000	0.00	04/30/15
g26133	pleiades	2014	056150.290	73.35	1439943.000	383792.710	81.40	04/30/15
g26134	pleiades	2014	18934.903	29.01	65278.000	46343.097	32.19	04/30/15
g26135	pleiades	2014	297536.708	92.98	319988.000	22451.292	103.19	04/30/15
g26137	pleiades	2014	443.122	0.22	202493.000	202049.878	0.24	04/30/15
g26141	pleiades	2014	34712.843	24.11	143995.000	109282.157	26.75	04/30/15
g26144	pleiades	2014	739301.919	97.92	754985.000	15683.081	108.67	04/30/15
g26146	pleiades	2014	18606.575	2.48	749970.000	731363.425	2.75	04/30/15
g26150	pleiades	2014	332100.700	72.07	460782.000	128681.300	79.98	04/30/15
g26153	pleiades	2014	652259.146	53.08	1228751.000	576491.854	58.91	04/30/15
g26158	pleiades	2014	0.000	0.00	4267.000	4267.000	0.00	04/30/15
g26159	pleiades	2014	10228.353	49.94	20480.000	10251.647	55.42	04/30/15
g26166	pleiades	2014	645165.481	97.76	659974.000	14808.519	108.49	04/30/15
g26171	pleiades	2014	162451.172	63.34	256490.000	94038.828	70.29	04/30/15
g26192	pleiades	2014	22080.390	9.58	230391.000	208310.610	10.64	04/30/15
g26197	pleiades	2014	457.911	3.58	12800.000	12342.089	3.97	04/30/15
g26202	pleiades	2014	1534606.890	97.15	1579651.000	45044.110	107.81	04/30/15
g26204	pleiades	2014	120873.861	16.12	749970.000	629096.139	17.89	04/30/15
g26209	pleiades	2014	1650577.060	45.27	3645688.000	1995110.940	50.24	04/30/15

Project	Host/Group	Fiscal Year	Used	% Used	Limit	Remain	Linear YTD Usage	Project Exp Date
g26123	pleiades	2015	435668.030	43.61	999100.000	563431.970	110.23	10/31/15
g26154	pleiades	2015	613.287	3.19	19200.000	18586.713	8.07	10/31/15
g26161	pleiades	2015	497979.510	55.29	2709100.000	1211120.490	139.77	10/31/15
g26164	pleiades	2015	21193.399	6.89	307800.000	286606.601	17.40	10/31/15
g26172	pleiades	2015	21692.517	6.04	359400.000	337707.483	15.26	10/31/15
g26179	pleiades	2015	676.709	61.52	1100.000	423.291	155.51	10/31/15
g26183	pleiades	2015	0.000	0.00	6400.000	6400.000	0.00	10/31/15
g26189	pleiades	2015	40944.287	14.33	285700.000	244755.713	36.23	10/31/15

Sample output from the "acct_ytd" job accounting utility showing updated information about usage on various Science Mission Directorate computing projects. Different fiscal year designations appear for projects that expire on different dates, and Linear YTD Usage number have been corrected for FY2015 projects

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Apple's OS X 10.10 Yosemite Deployed to Staff Workstations *

- The NASA Advanced Supercomputing (NAS) Division's Engineering Servers and Services (ESS) team completed development of a Yosemite image ready to deploy on 200 Mac systems used by staff at the NAS facility.
- Once the image passed a NAS security scan and was approved by the NASA Ames Exploration Technology Directorate's security official, the ESS team began deployment to beta users to further validate the deployment.
- Preparation work for the Yosemite rollout included: creating disk and netboot images; upgrading cfengine 2 to version 3; converting to network packet filters and enabling the firewall; testing all software, and overcoming issues with Keymaster, KACE, Entrust, Symantec antivirus and Java.
- Improvements in account creation during the system deployments allow the ESS team to do data restores and application loading synchronously, resulting in upgrades that take several hours less than Mavericks upgrades.

Mission Impact: Apple's annual release of a major operating system (OS) makes it a challenge for enterprise sites to stay current and run the latest hardware/software configuration. The Yosemite upgrade allows HECC to run the latest OS and support the latest hardware for scientific users and staff.

Apple's OS X 10.10 (Yosemite) system was released in October 2014, and is required for the latest MacBook Pro laptops.

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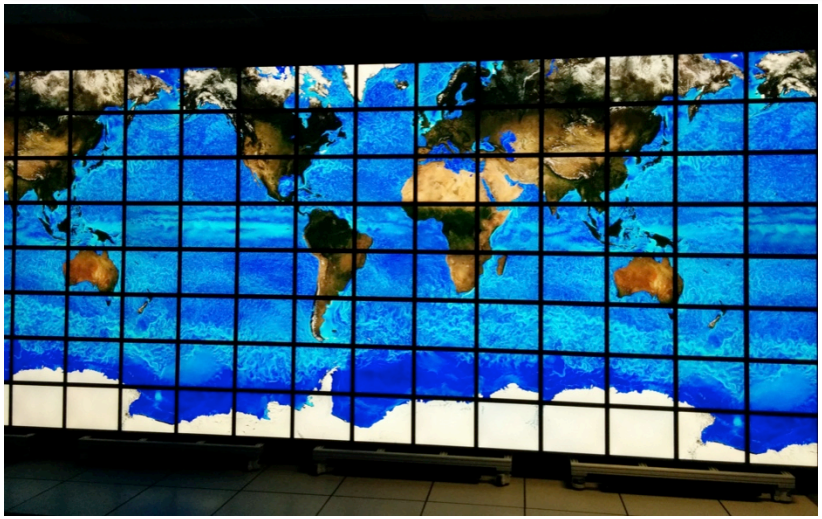
** HECC covers only a portion of this cost*

Pleiades-Run Simulations Provide A Virtual Telescope on the World's Oceans and Sea Ice *

- Researchers with the Estimating the Circulation and Climate of the Ocean (ECCO) consortium are running simulations on Pleiades to produce global "maps" of Earth's ocean and sea-ice system at an unprecedented resolution (~1 km horizontal grid).
- The simulations are produced with the Massachusetts Institute of Technology general circulation model (MITgcm) on up to 70,000 Pleiades cores, and are compared to observational data from NASA satellites, ocean sensors, and ship-borne and mooring data.
- The resulting output provides the oceanic equivalent of a telescope that can reveal the state of the entire ocean/sea-ice system in exceptional detail. Researchers can use this modeling tool to:
  - Investigate fundamental questions such as how the circulation, chemistry, and biology of the ocean collectively interact with atmospheric carbon.
  - Determine how a pollutant plume or debris field might spread from a particular ocean location, or where and when heat is absorbed by or released from the ocean.
- As HECC storage capabilities continue to increase, this work can potentially develop into a transformative strategy for understanding and predicting the impact of global ocean circulation on climate.

Mission Impact: HECC resources enable high-resolution global simulations that help researchers monitor ocean, sea-ice, and atmospheric systems to learn how they interact and evolve, and to better understand their impact on climate.



The full display resolution (25,600 x 9,600 pixels) of the NAS facility's hyperwall is required to view the output of this ECCO ocean simulation. HECC visualization experts developed the ability to navigate through multiple layers of the simulation to examine scalar and vector fields at various ocean depths. *David Ellsworth and Chris Henze, NASA/Ames*

POCs: Chris Hill, cnh@mit.edu, (617) 253-6430, Massachusetts Institute of Technology; Dimitris Menemenlis, dimitris.menemenlis@jpl.nasa.gov, (818) 354-1656, NASA Jet Propulsion Laboratory

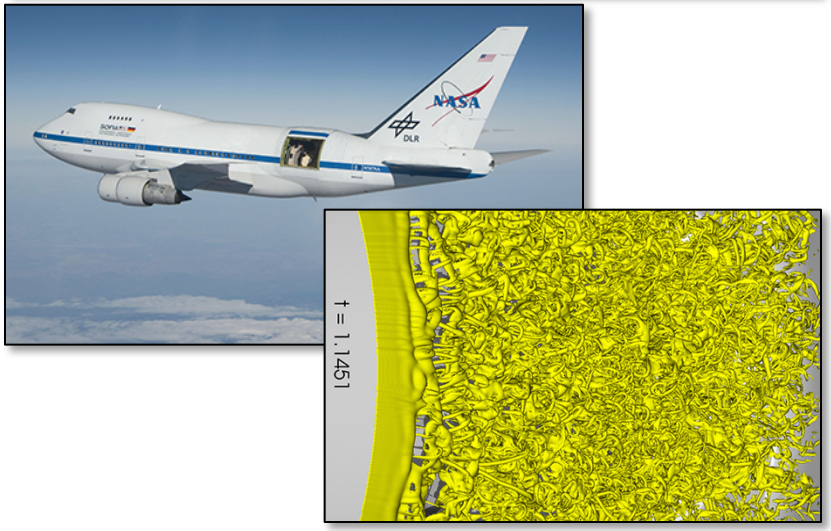
** HECC provided supercomputing resources and services in support of this work*

Simulation and Analysis of SOFIA Telescope Cavity Acoustics Enabled by Pleiades *

- Researchers performed unique computational fluid dynamics (CFD) simulations on Pleiades to investigate unsteady flow physics and noise generation in the telescope cavity of the Stratospheric Observatory for Infrared Astronomy (SOFIA) aircraft.
- To efficiently model the complex, multi-scale geometry and unsteady flows, the research team:
  - Used NASA ARC's Launch Ascent and Vehicle Aerodynamics (LAVA) CFD code to assess how the unsteady flow field inside and over the cavity interferes with the optical path and mounting of the telescope.
  - Performed implicit large-eddy simulations using LAVA's temporally 4th-order-accurate Runge-Kutta scheme and spatially 5th-order WENO-5Z scheme.
  - Used LAVA's immersed boundary method, coupled with a block-structured Cartesian adaptive mesh refinement framework, to automate generation of computational grids for the complex geometries.
- Results focused on how the unsteady flow field inside and over the open cavity may contribute to structural vibrations of the telescope.
- Strong scaling studies showed that simulations with 4 billion computational cells scale excellently using up to 32,000 cores on Pleiades, enabling one-week turnaround of many grid solutions—15 years ago, the same work would have taken 6 months.

** HECC provides supercomputing resources and services in support of this work*

Mission Impact: Simulations enabled by the Pleiades supercomputer helped identify important mechanisms that could affect the image clarity of the telescope aboard the Stratospheric Observatory for Infrared Astronomy (SOFIA) telescope.



Top: The SOFIA aircraft, showing the open aft cavity where a 2.5-meter infrared telescope is mounted. Bottom: Image from a simulation showing vorticity contours in the shear layer at the telescope cavity opening. Vorticity measures the level of rotation in the flow, and is used to identify coherent flow structures. Flow is from left to right. *Michael Barad, NASA/ Ames*

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HECC Facility Hosts Several Visitors and Tours in March 2015

- HECC hosted 7 tour groups in March; guests learned about the agency-wide missions being supported by HECC assets, and some of the groups also viewed the D-Wave Two quantum computer system. Visitors this month included:
  - Jason Wong, Associate Director, Office of Naval Research Global in Tokyo, visited the NAS facility as part of his Ames tour.
  - Andy David, Consul General to the Pacific Northwest, Israel; this first-time visit to Ames was planned to support ongoing collaborations with Israel and is key to building goodwill, leading to further activities in the future.
  - Ahmed F. Ghoniem, Director of the Center for Energy and Propulsion Research at Massachusetts Institute of Technology, toured the facility after his technical presentation as part of the NAS Division's Applied Modeling and Simulation series.
  - 23 graduate students from Mines ParisTech Graduate School in France made a visit to Ames and toured the NAS facility.
  - Six female high school sophomores from the Castilleja School in Palo Alto, CA toured the facility as part of a "career day" visit to Ames.

A student group examines scientific visualizations displayed on the hyperwall system during a visit to the NASA Advanced Supercomputing (NAS) facility.

POC: Gina Morello, gina.f.morello@nasa.gov, (650) 604-4462, NASA Advanced Supercomputing Division

Papers and Presentations

- "**Three-Dimensional Analytical Description of Magnetized Winds from Oblique Pulsars**," A. Tchekhovskoy, et. al., arXiv:1503.01467 [astro-ph.HE], March 4, 2015. * *http://arxiv.org/abs/1503.01467*
- "**Powerful Radiative Jets in Super-Critical Accretion Disks Around Non-Spinning Black Holes**," A. Sadowski, R. Narayan, arXiv:1503.00654 [astro-ph.HE], March 2, 2015. * *http://arxiv.org/abs/1503.00654*
- "**Aerodynamic Shape Optimization with Goal-Oriented Error Estimation and Control**," M. Nemec, presented at the SIAM Computing Science & Engineering Conference, Salt Lake City, UT, March 17, 2015.
- "**M2 Proton Channel: Toward a Model of a Primitive Proton Pump**," C. Wei, A. Pohorille, Origins of Life and Evolution of Biospheres, Springer, March 17, 2015. * *http://link.springer.com/article/10.1007/s11084-015-9421-x*
- "**Implementing Marine Organic Aerosols into the GEOS-Chem Model**," B. Gantt, et. al., Geosci. Model Dev., 8, 619-629, March 17, 2015. * *http://www.geosci-model-dev.net/8/619/2015/gmd-8-619-2015.html*
- "**Planes of Satellite Galaxies and the Cosmic Web**," N. Libeskind, et. al., arXiv: 1503.05915 [astro-ph.GA], March 19, 2015. * *http://arxiv.org/abs/1503.05915*

** HECC provided supercomputing resources and services in support of this work*

Papers and Presentations (cont.)

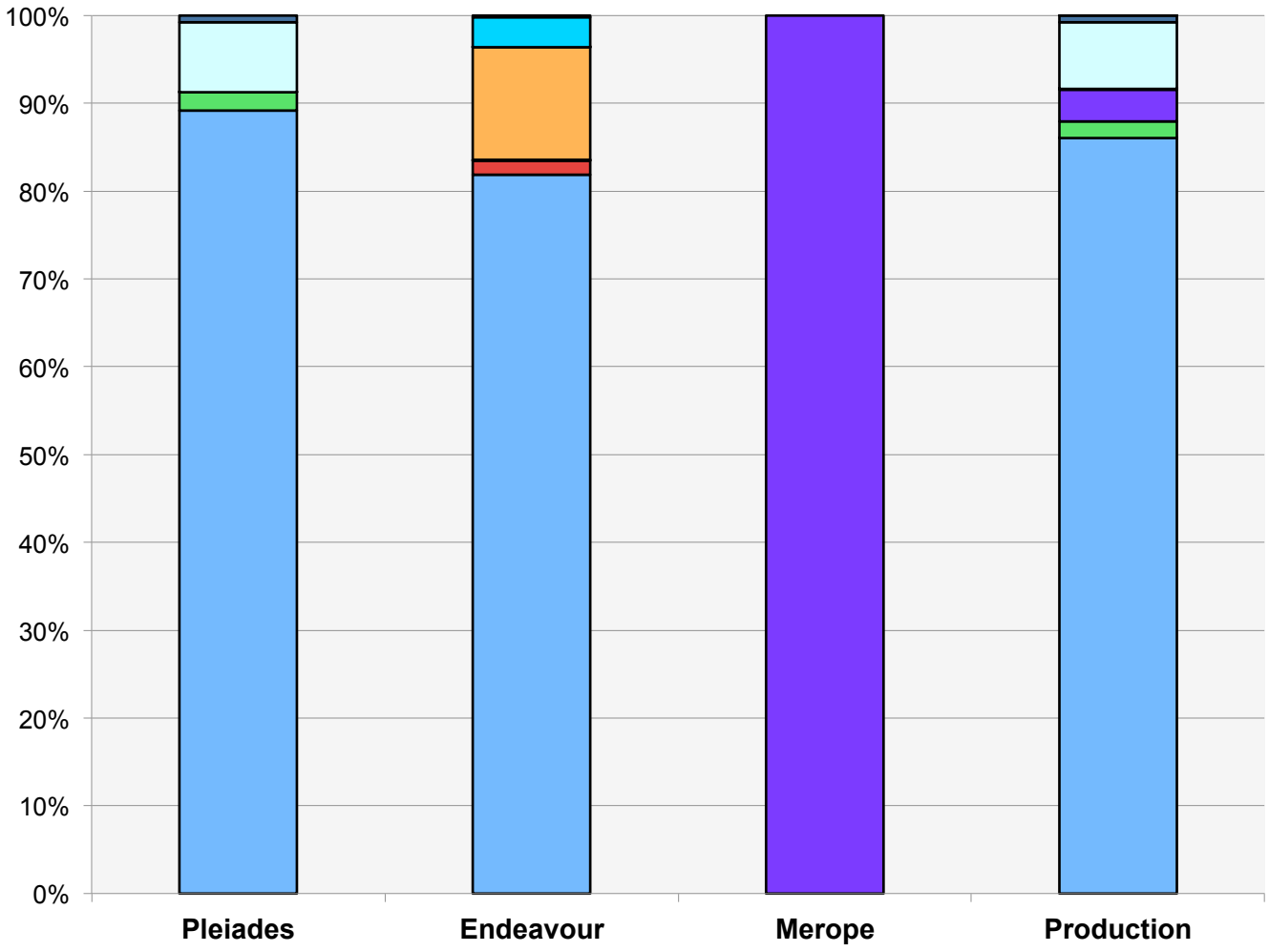
- "**Determination and Correction of Persistent Biases in Quantum Annealers**," A. Perdomo-Ortiz, et. al., arXiv:1503.05679 [astro-ph], March 19, 2015. * *http://arxiv.org/abs/1503.05679*
- "**Caught in the Act: Gas and Stellar Velocity Dispersions in a Fast Quenching Compact Star-Forming Galaxy at z~1.7**," G. Barro, et. al., arXiv:1503.07164 [astro-ph.GA], March 24, 2015. * *http://arxiv.org/abs/1503.07164*
- **ARC-LaRC Performance Characterization Meeting**—presenter: Dan Kokron, March 24, 2015.

** HECC provided supercomputing resources and services in support of this work*

News and Events

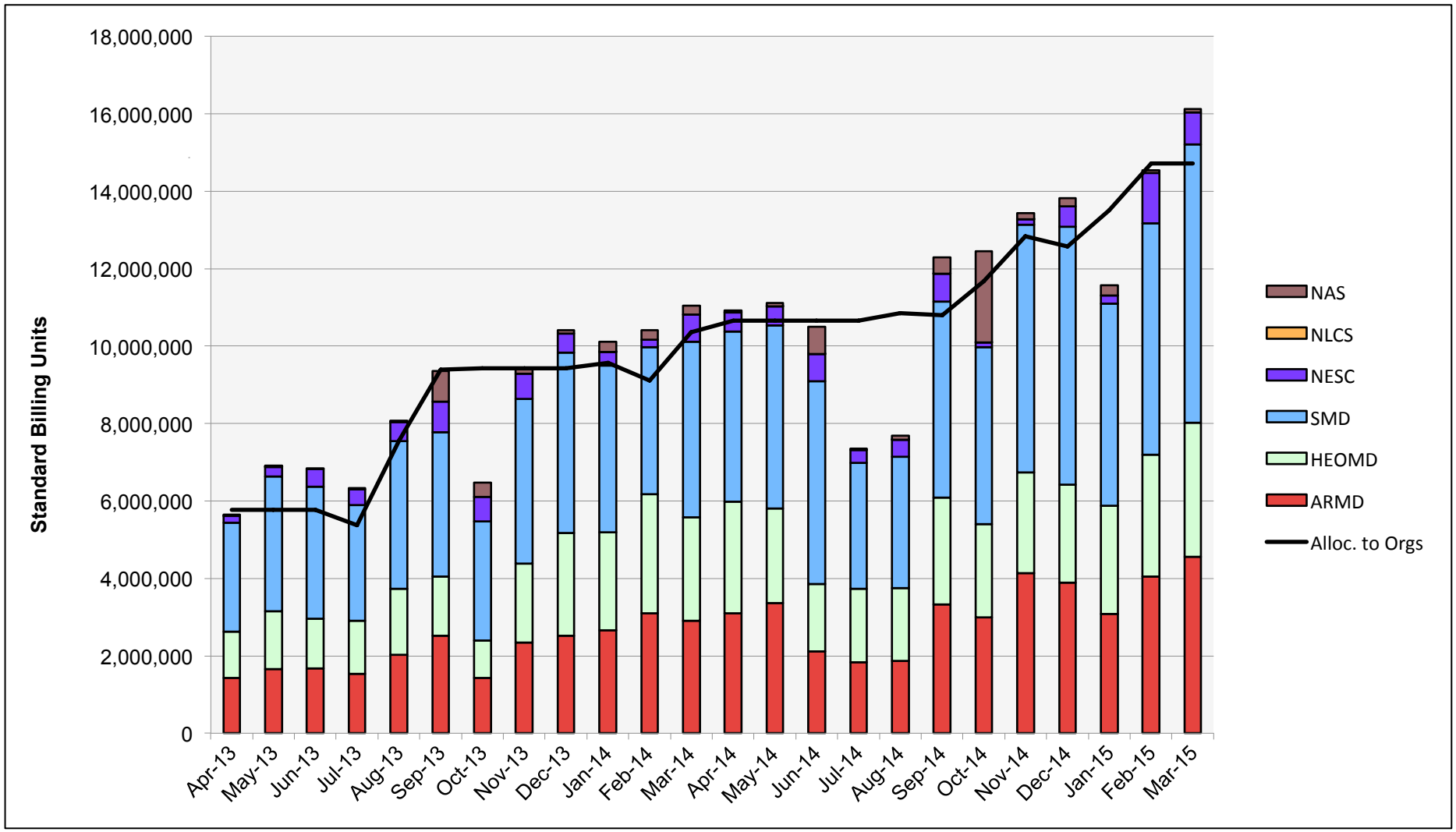
- **NASA-Funded Study Finds Two Solar Wind Jets in the Heliosphere**, *NASA Goddard Press Release*, March 3, 2015—Researchers utilized the Pleiades supercomputer to run simulations of the heliosphere and discovered that it was smaller than previously thought. *http://www.nasa.gov/content/goddard/two-solar-wind-jets-found-in-the-heliosphere*
- **Race to Find the First Exomoon Heats Up**, *New Scientist*, March 17, 2015—A team led by David Kipping at the Harvard-Smithsonian Center for Astrophysics is searching for exomoons by modeling all the positions one could be in and looking for similar light signals in the Kepler data, using Pleiades to crunch the numbers. *http://www.newscientist.com/article/dn27180-race-to-find-the-first-exomoon-heats-up.html*
  - **Searching for the First Exomoon, with the Help of Supercomputers**, *Extreme Tech*, March 18, 2015. *http://www.extremetech.com/extreme/201458-searching-for-the-first-exomoon-with-the-help-of-supercomputers*
  - **Astronomers On the Hunt for Exomoons That May Host Alien Life**, *Space.com*, March 25, 2015. *http://www.space.com/28918-exomoons-alien-life-search.html*
  - **Hunting for Exomoons That May Host Alien Life**, *Discovery News*, March 30, 2015. *http://news.discovery.com/space/alien-life-exoplanets/hunting-for-exomoons-that-may-host-alien-life-150330.htm*

HECC Utilization

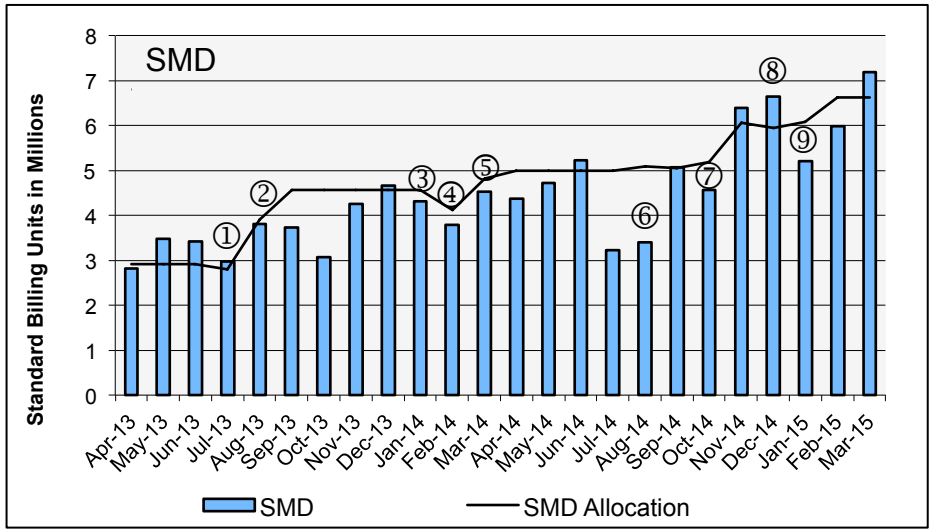


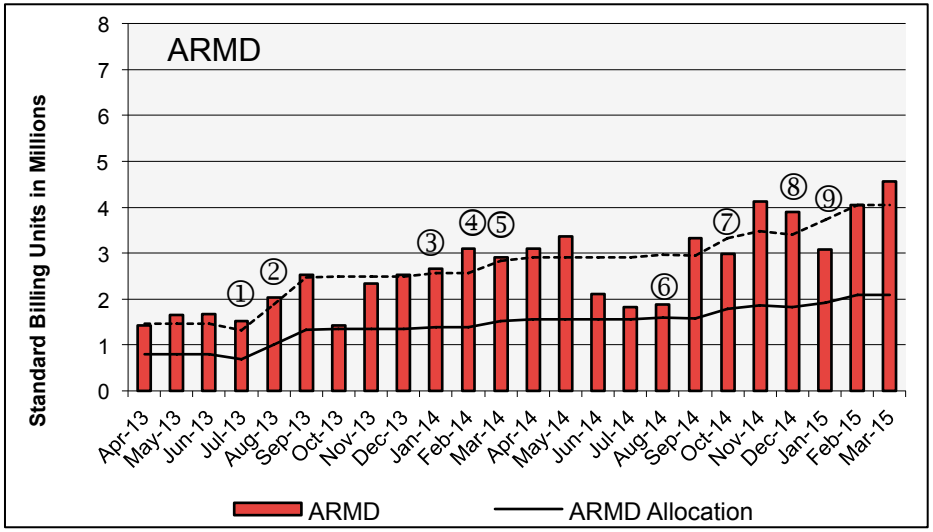
March 2015

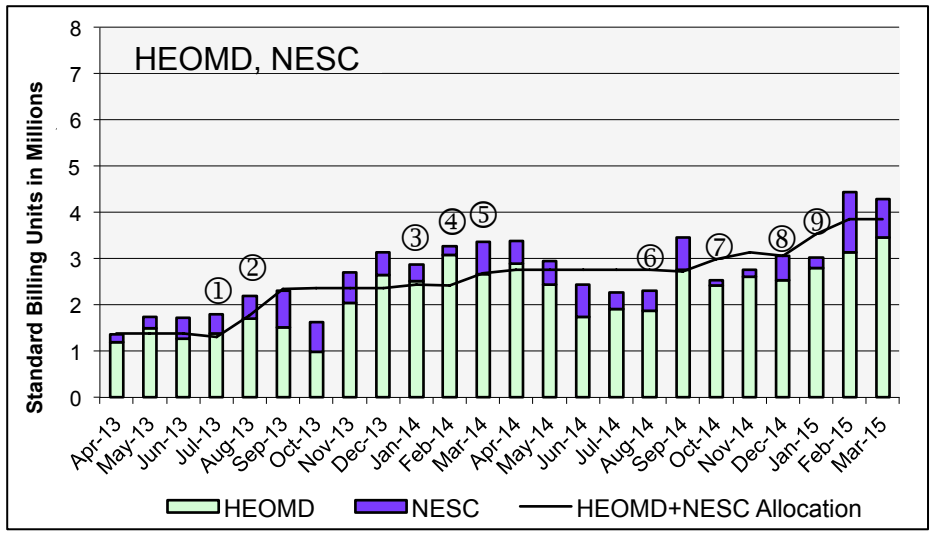
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month







① 32 Harpertown Racks retired

② 32 Harpertown Racks retired; 46 Ivy Bridge Racks added

③ 6 Ivy Bridge Racks added; 20 Nehalem, 12 Westmere Racks Retired

④ 8 Ivy Bridge Racks added mid-Feb; 8 Ivy Bridge Racks added late Feb.

⑤ 4 Ivy Bridge Racks added mid-March

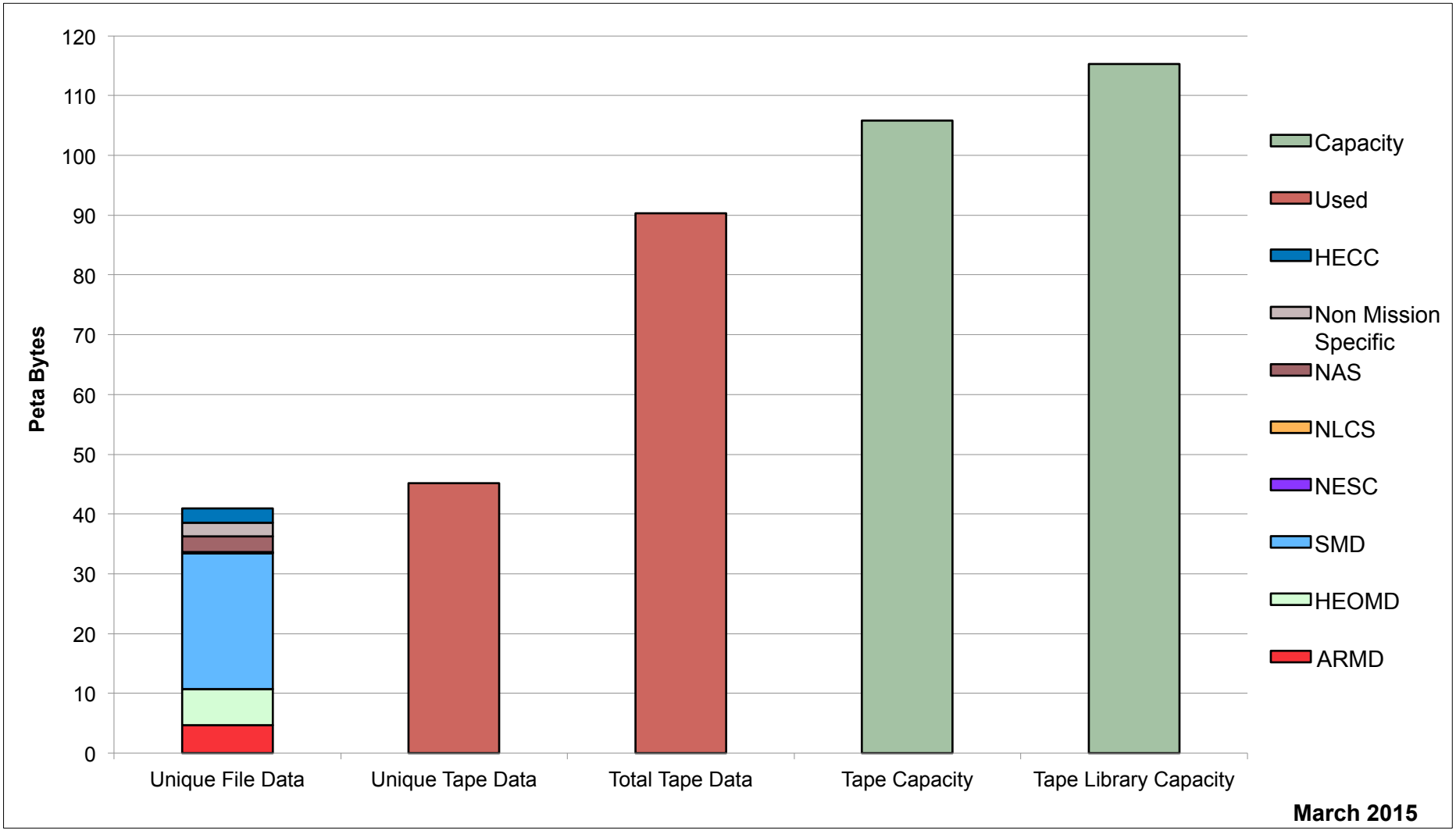
⑥ 6 Westmere Racks added to Merope, Merope Harpertown retired

⑦ 16 Westmere Racks retired; 10 Nehalem Racks and 2 Westmere Racks added to Merope; 3 Ivy Bridge Racks added; 15 Haswell Racks added

⑧ 16 Westmere Racks retired

⑨ 14 Haswell racks added

Tape Archive Status



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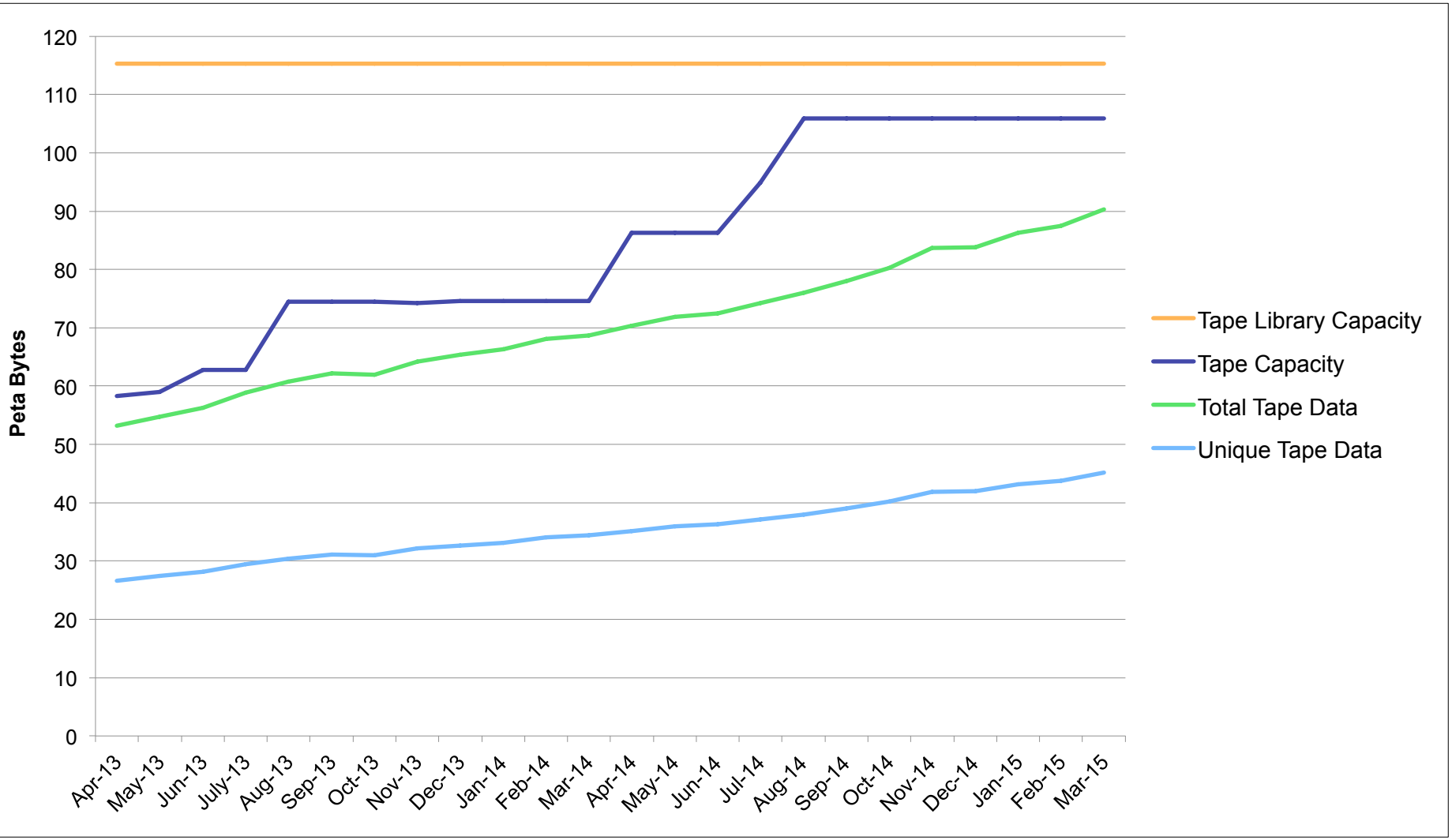
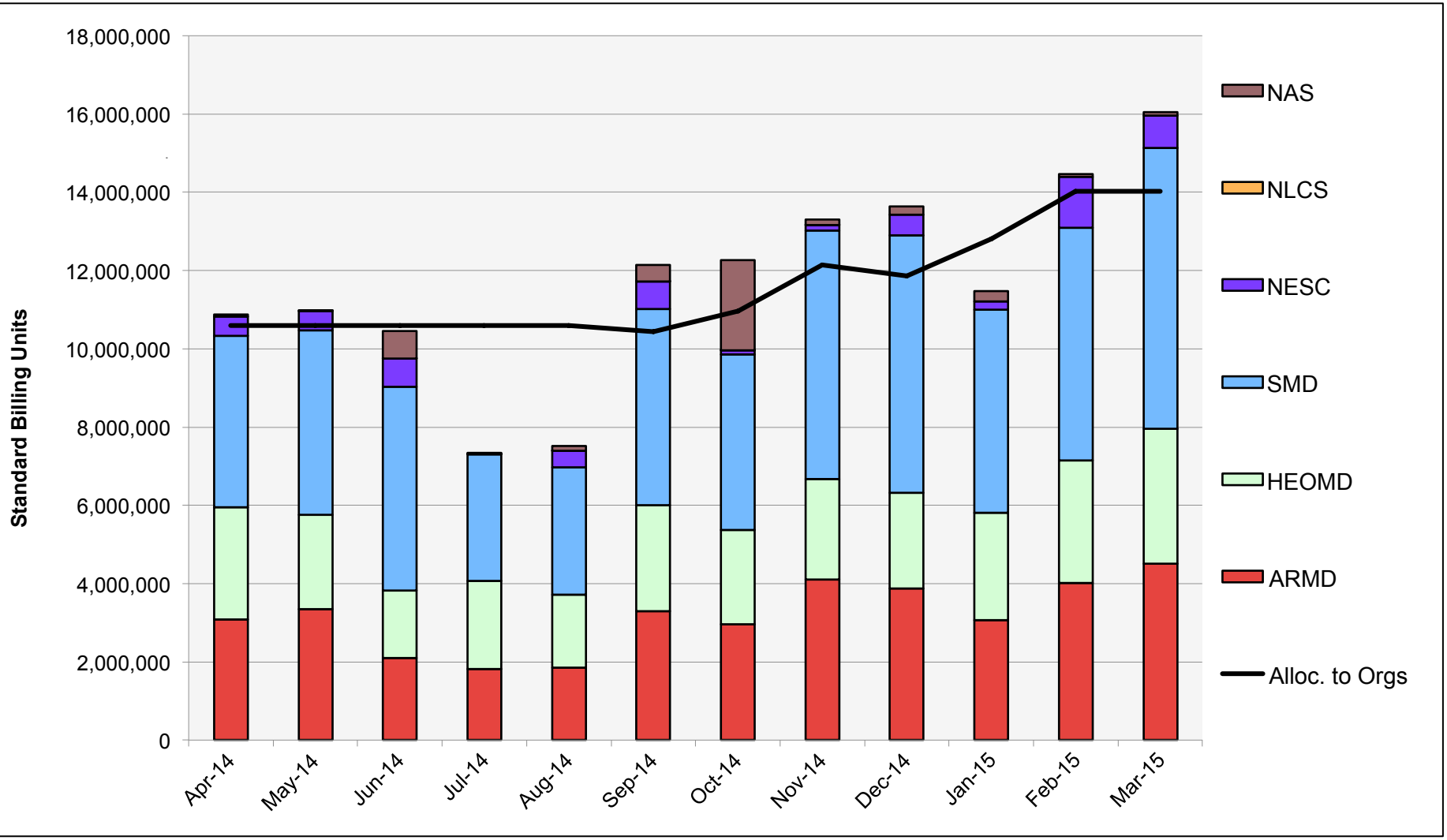
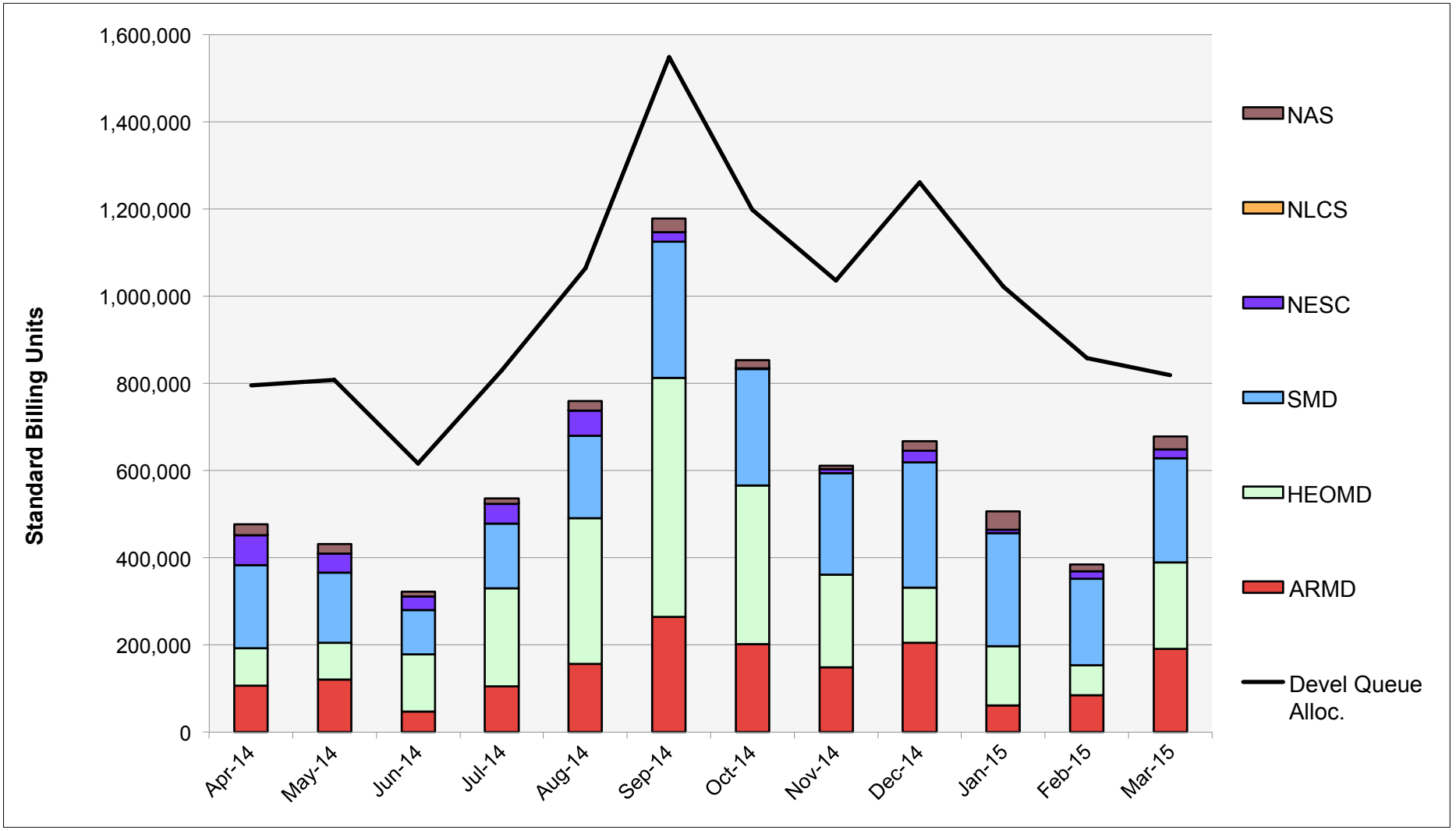


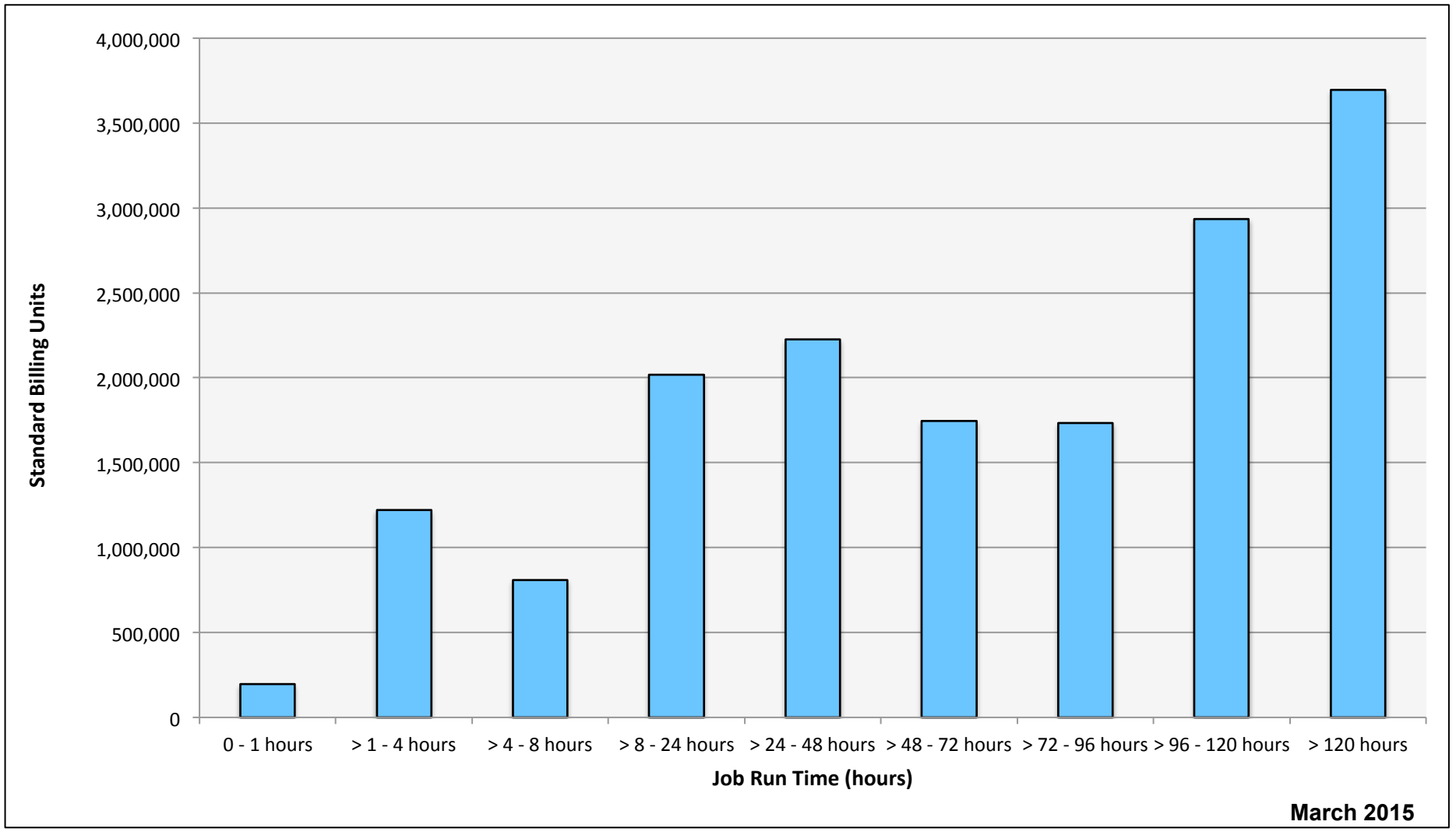
Pleiades:
SBUs Reported, Normalized to 30-Day Month



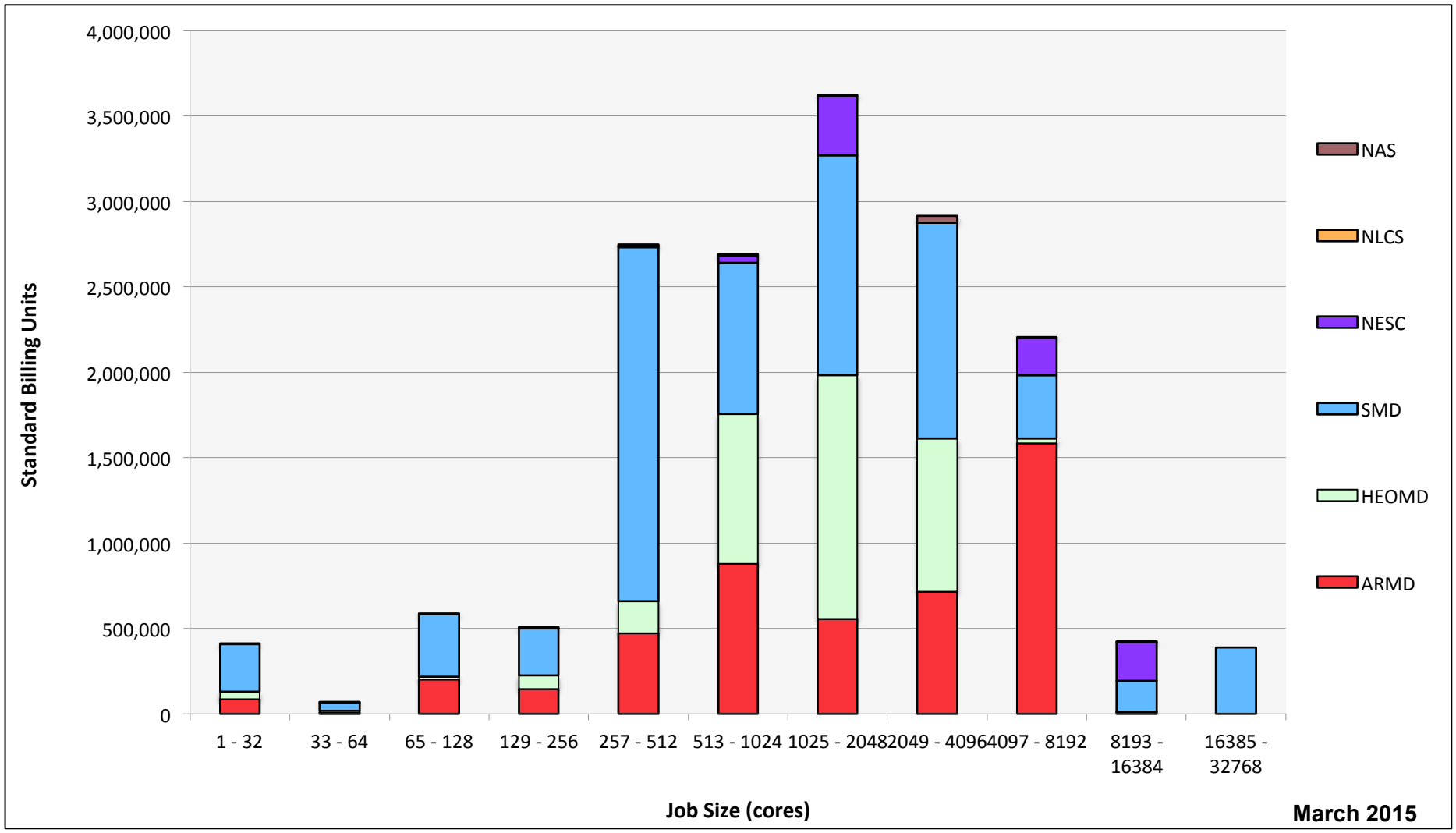
Pleiades:
Devel Queue Utilization



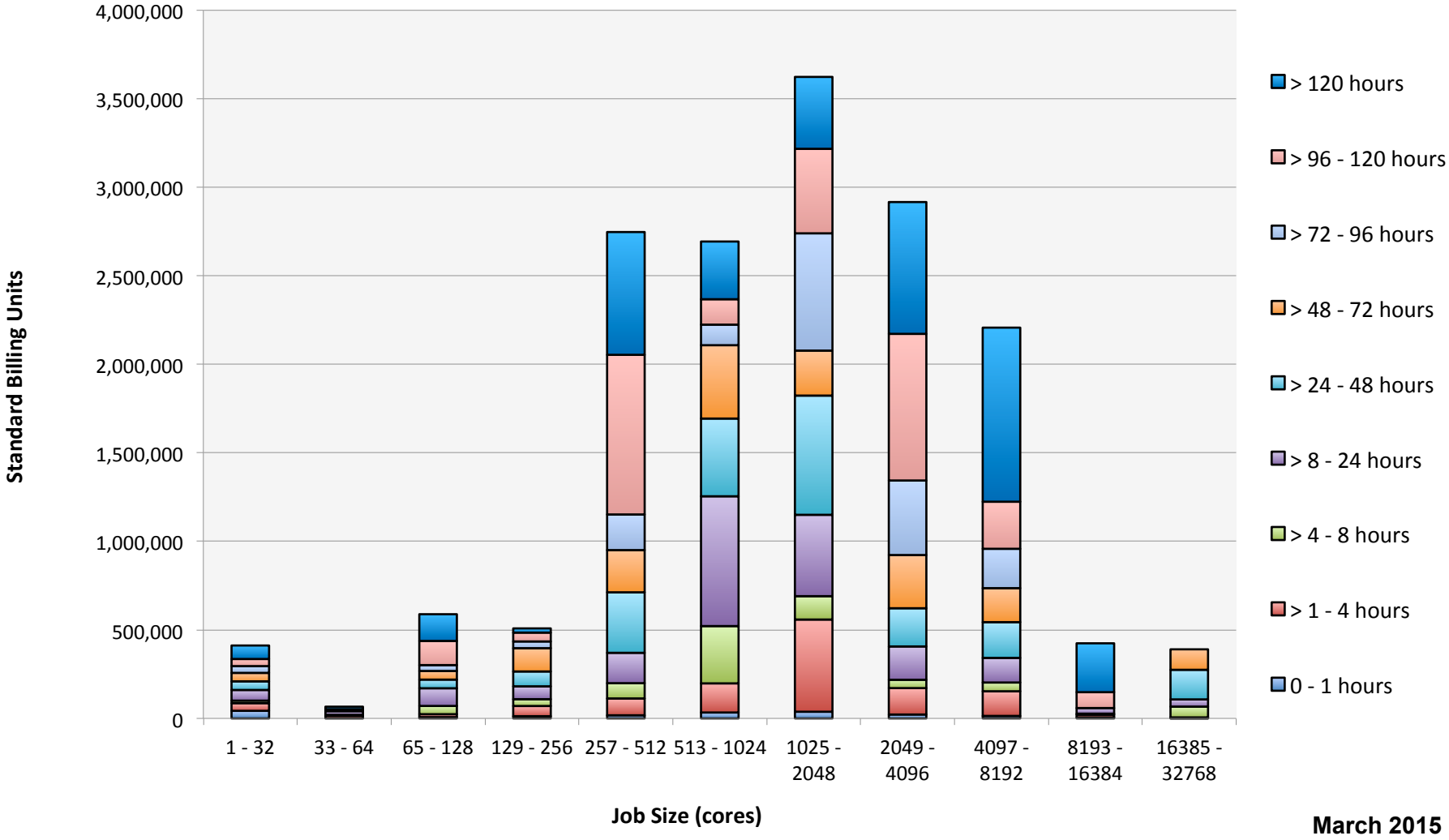
Pleiades:
Monthly Utilization by Job Length



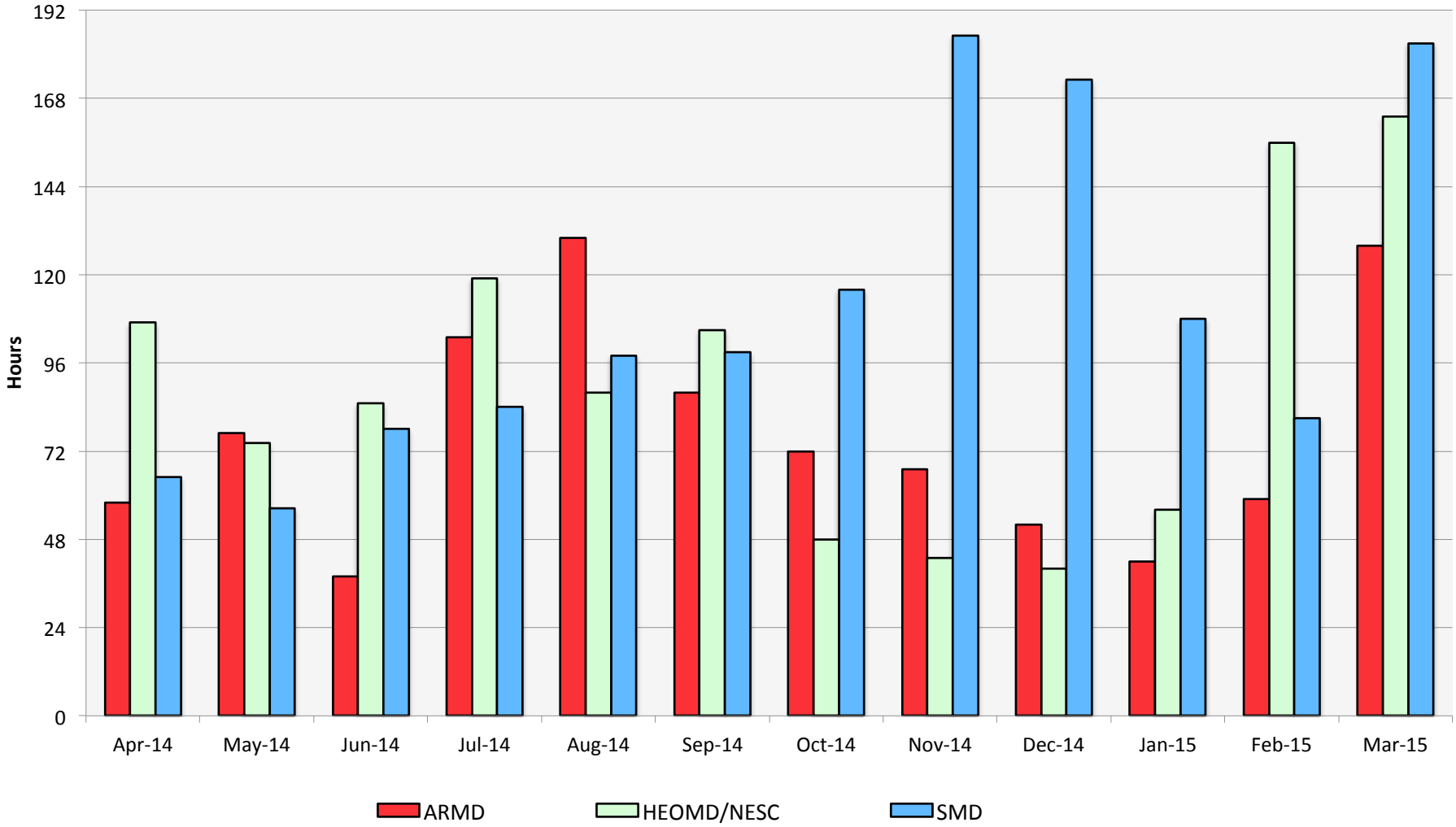
Pleiades:
Monthly Utilization by Size and Mission



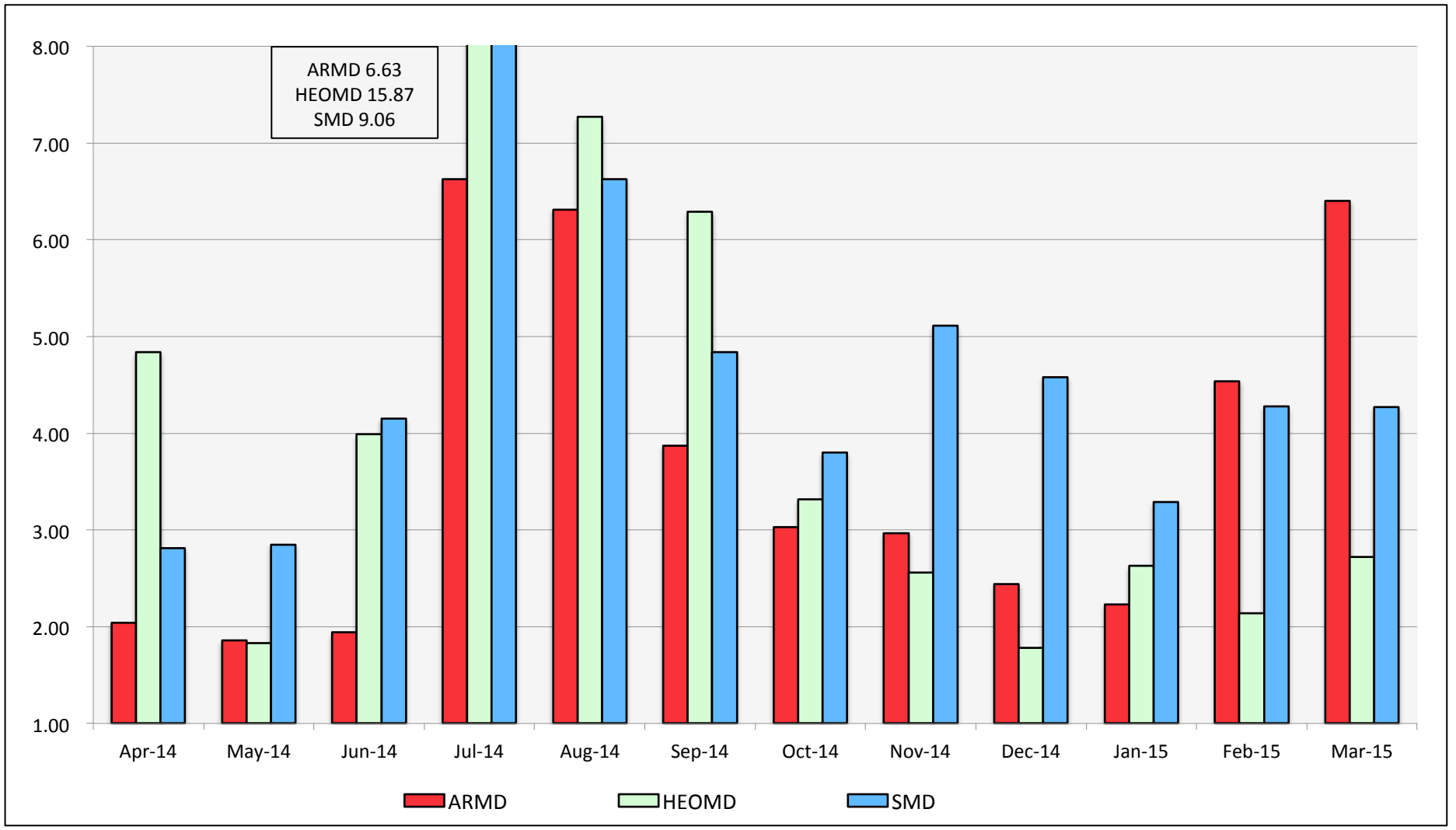
Pleiades:
Monthly Utilization by Size and Length



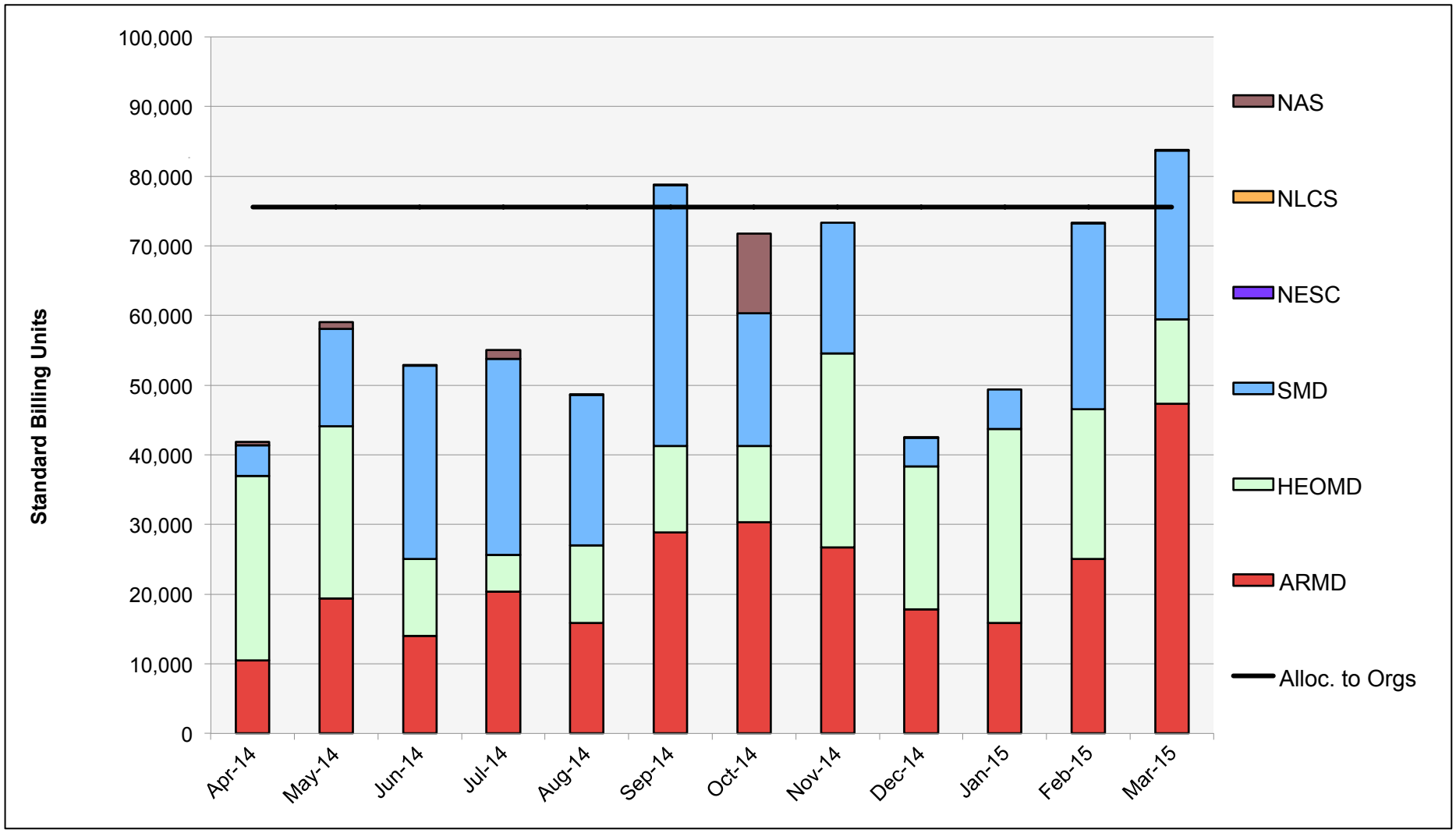
Pleiades:
Average Time to Clear All Jobs



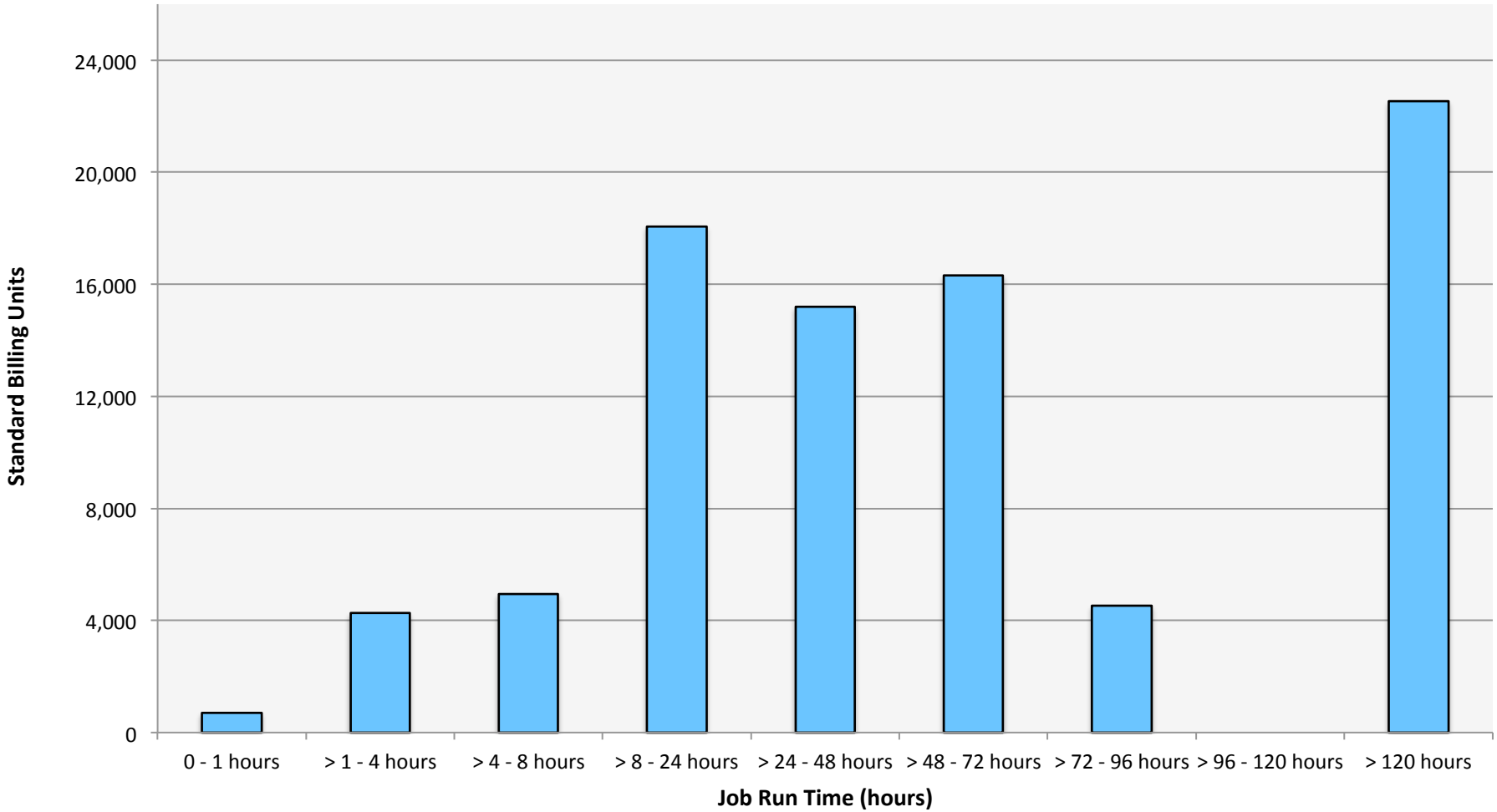
Pleiades:
Average Expansion Factor



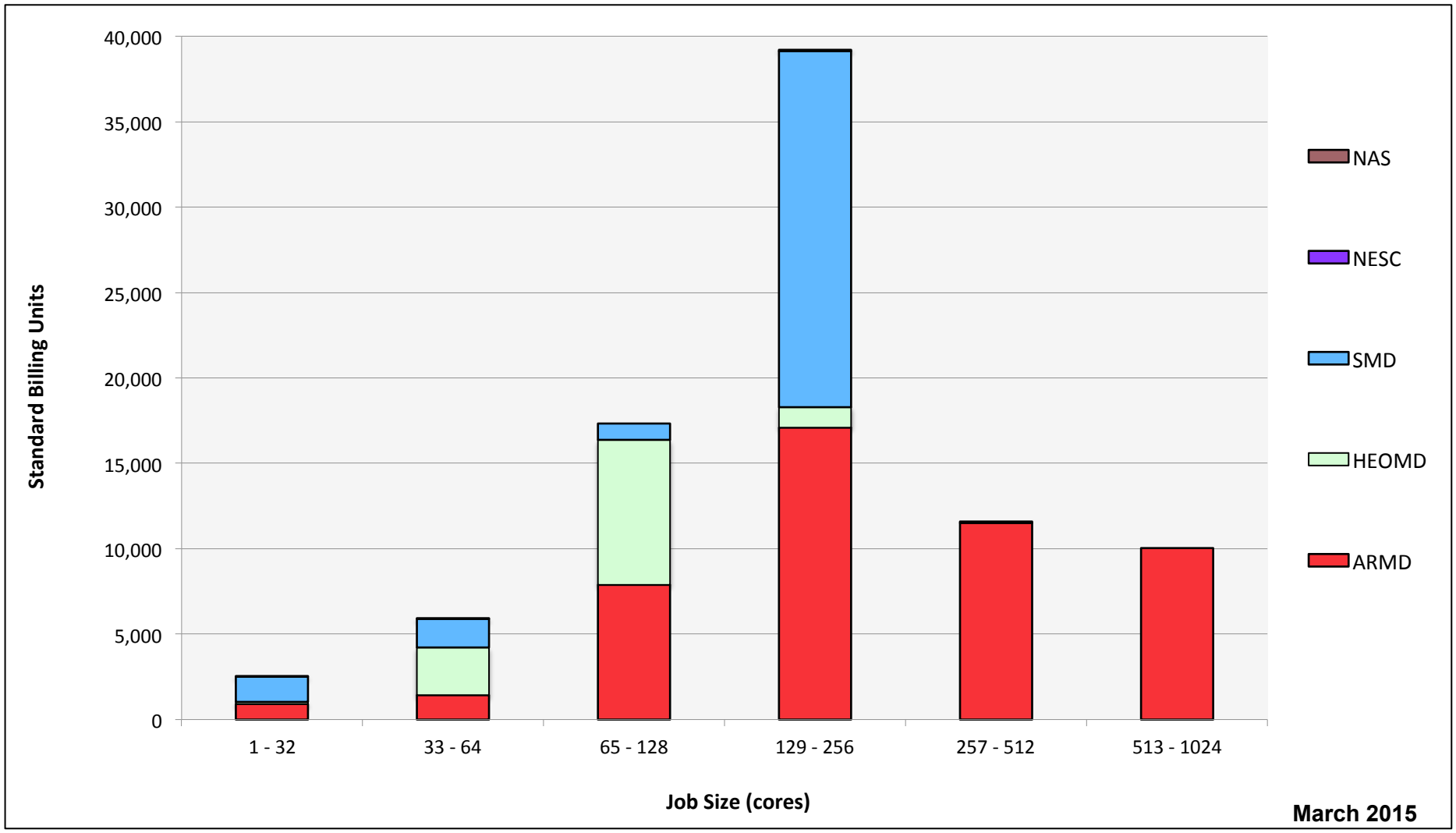
Endeavour:
SBUs Reported, Normalized to 30-Day Month



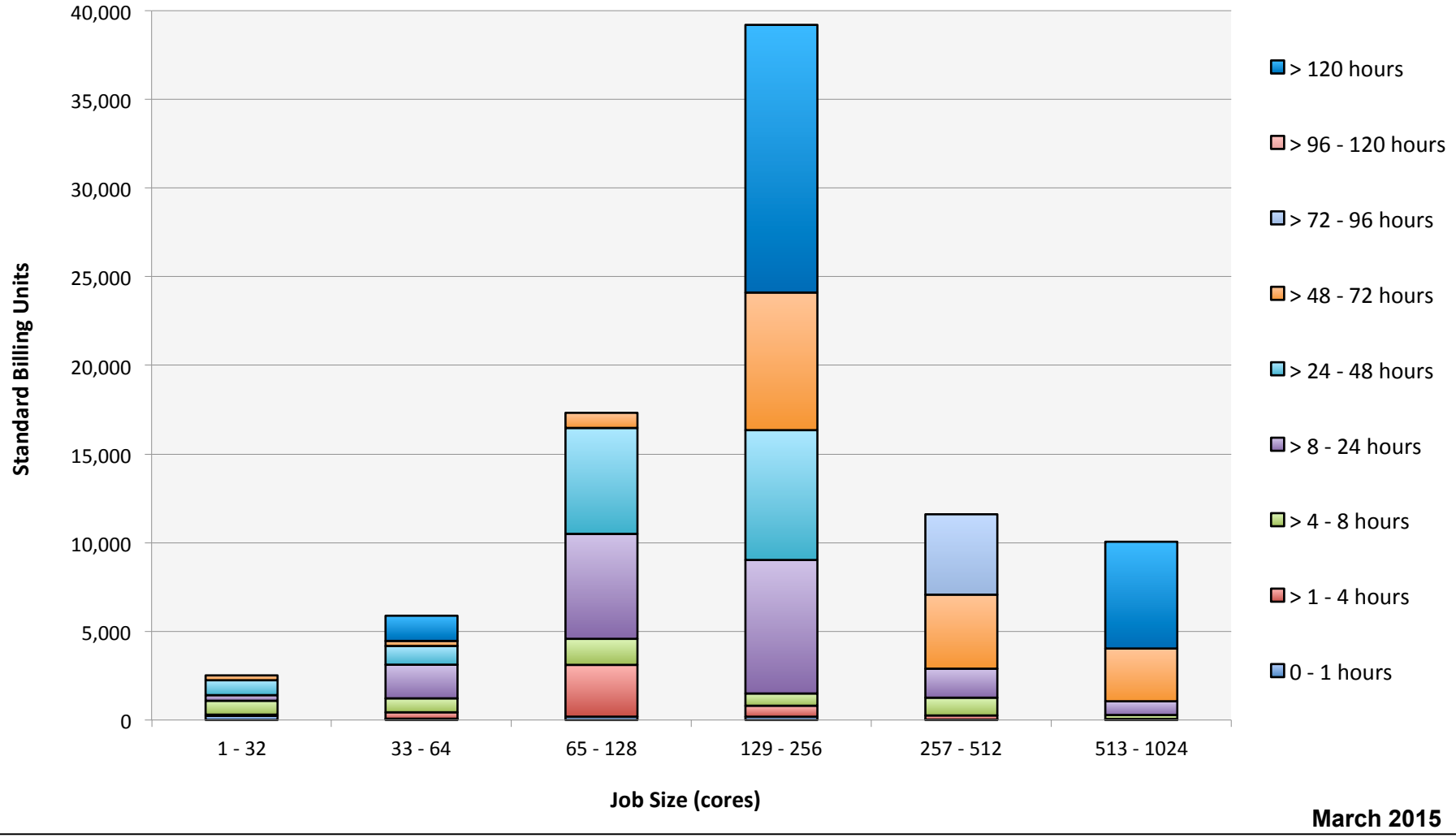
Endeavour:
Monthly Utilization by Job Length



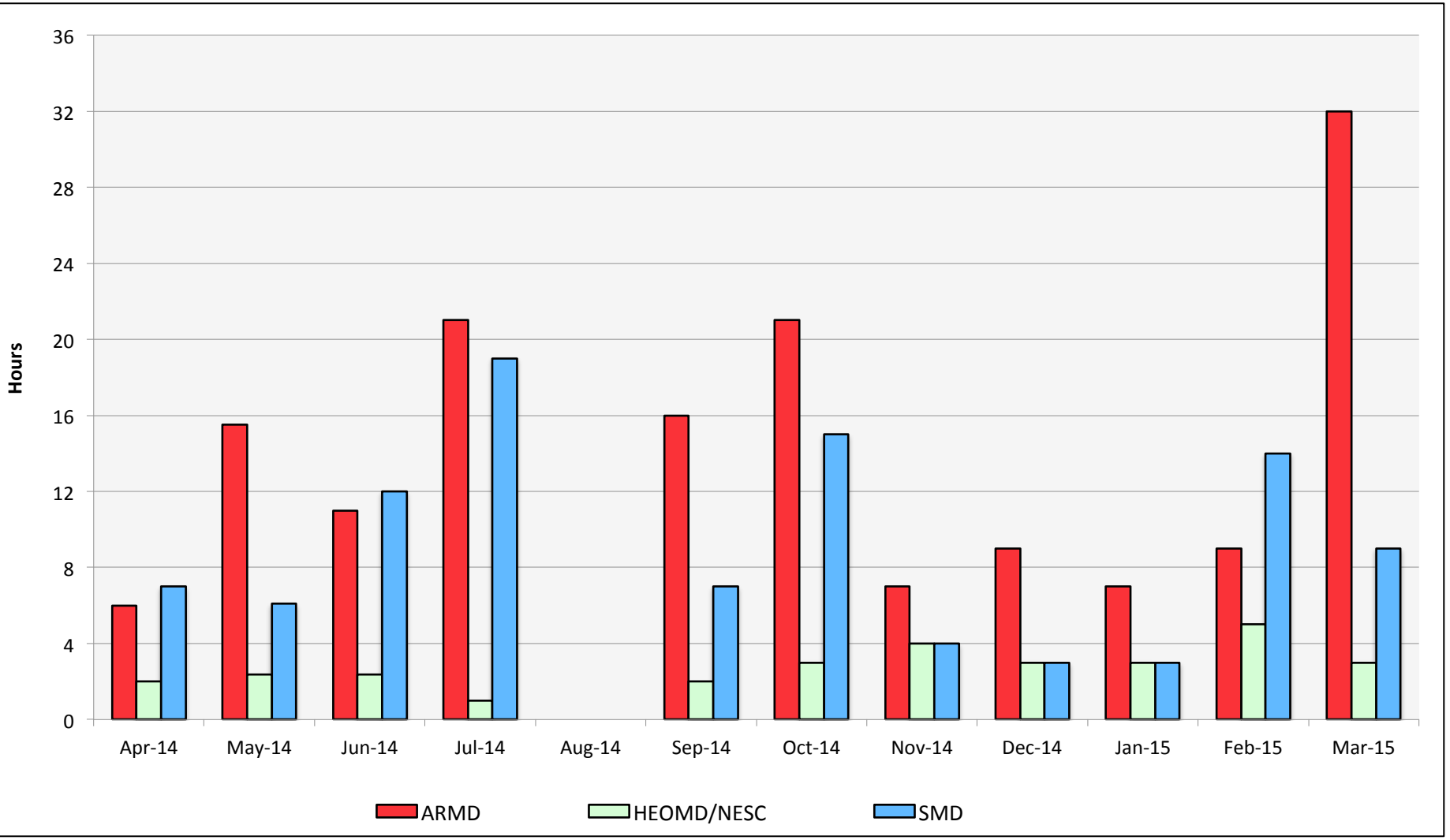
Endeavour:
Monthly Utilization by Size and Mission



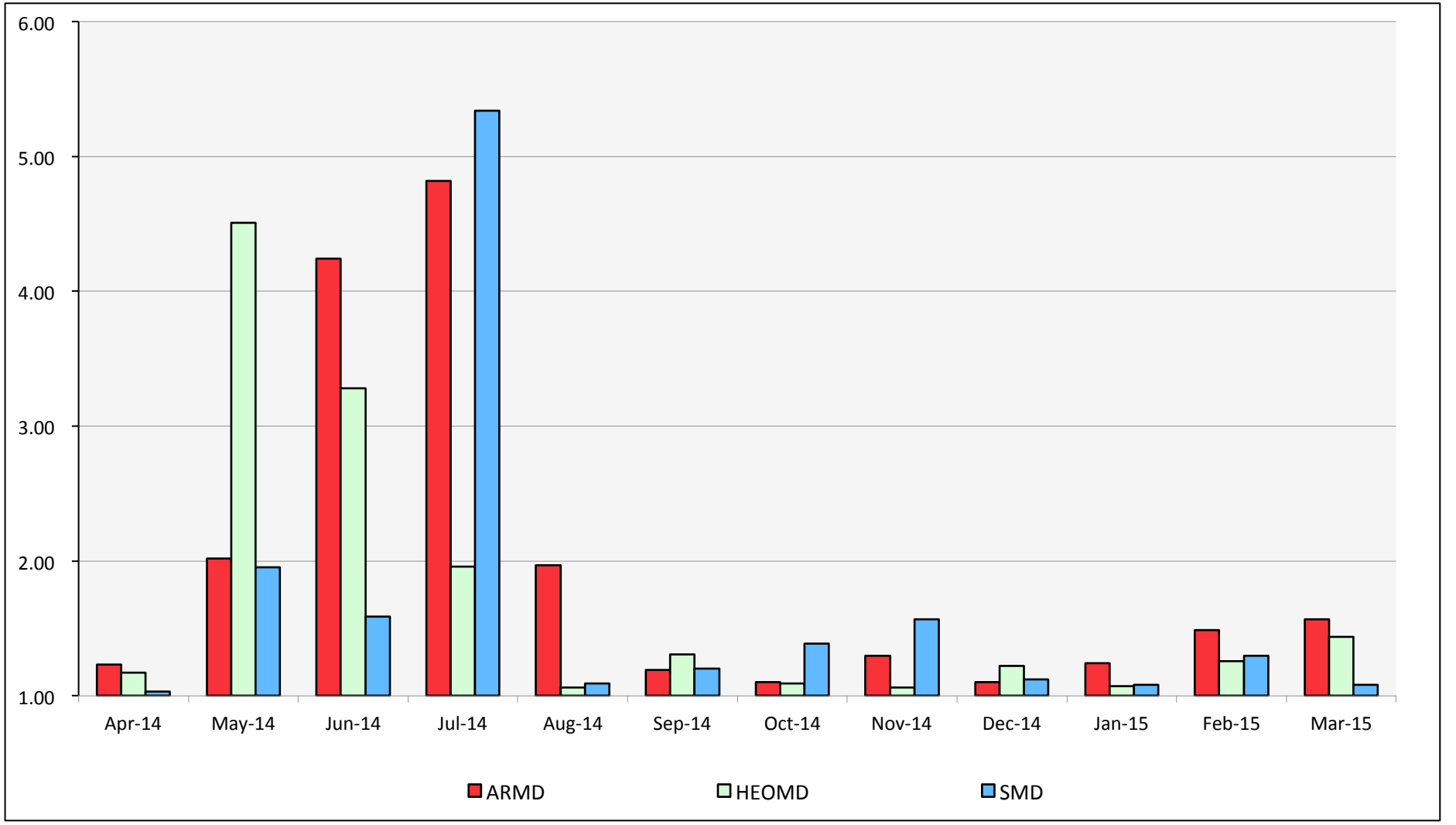
Endeavour:
Monthly Utilization by Size and Length



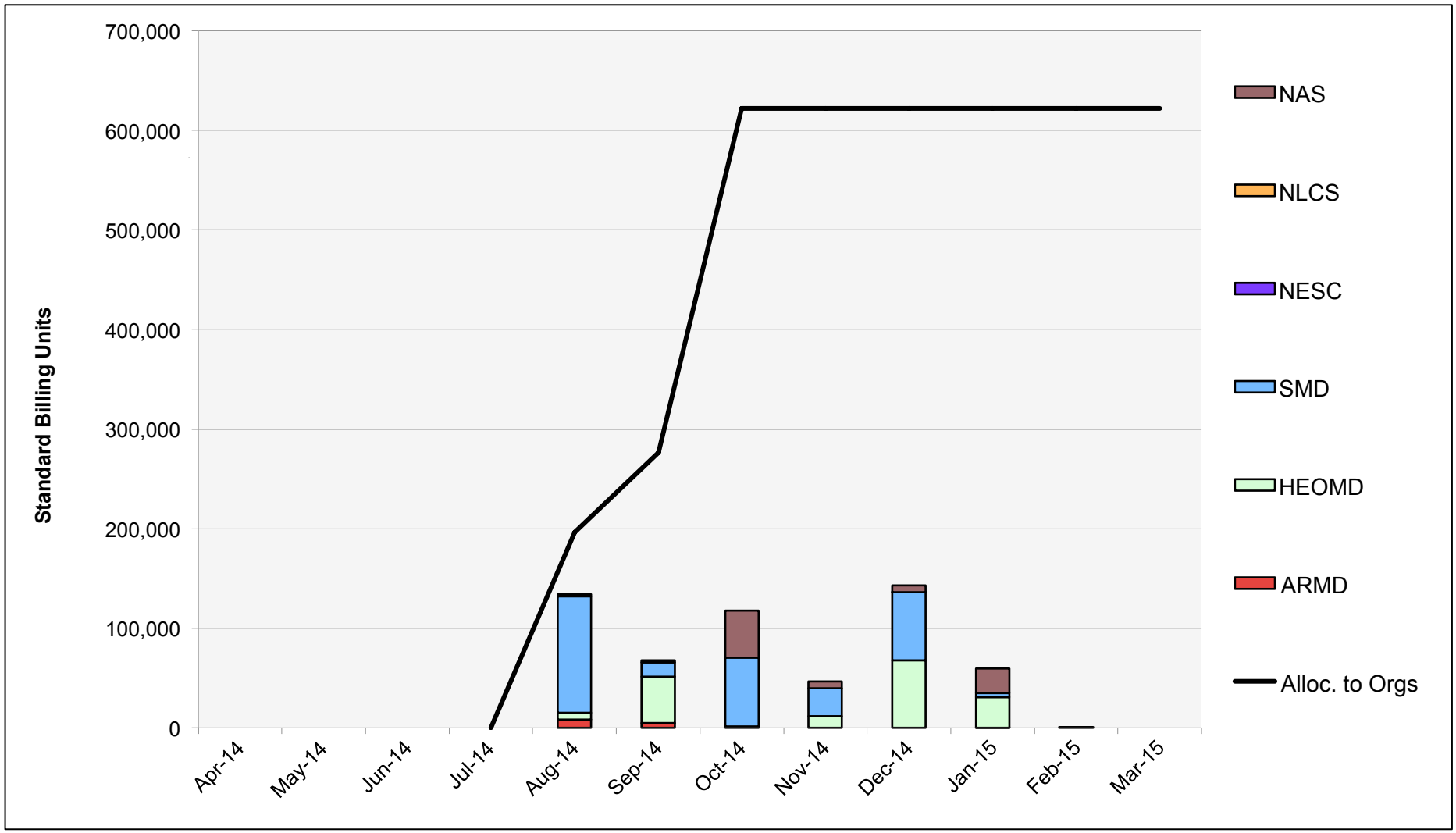
Endeavour:
Average Time to Clear All Jobs



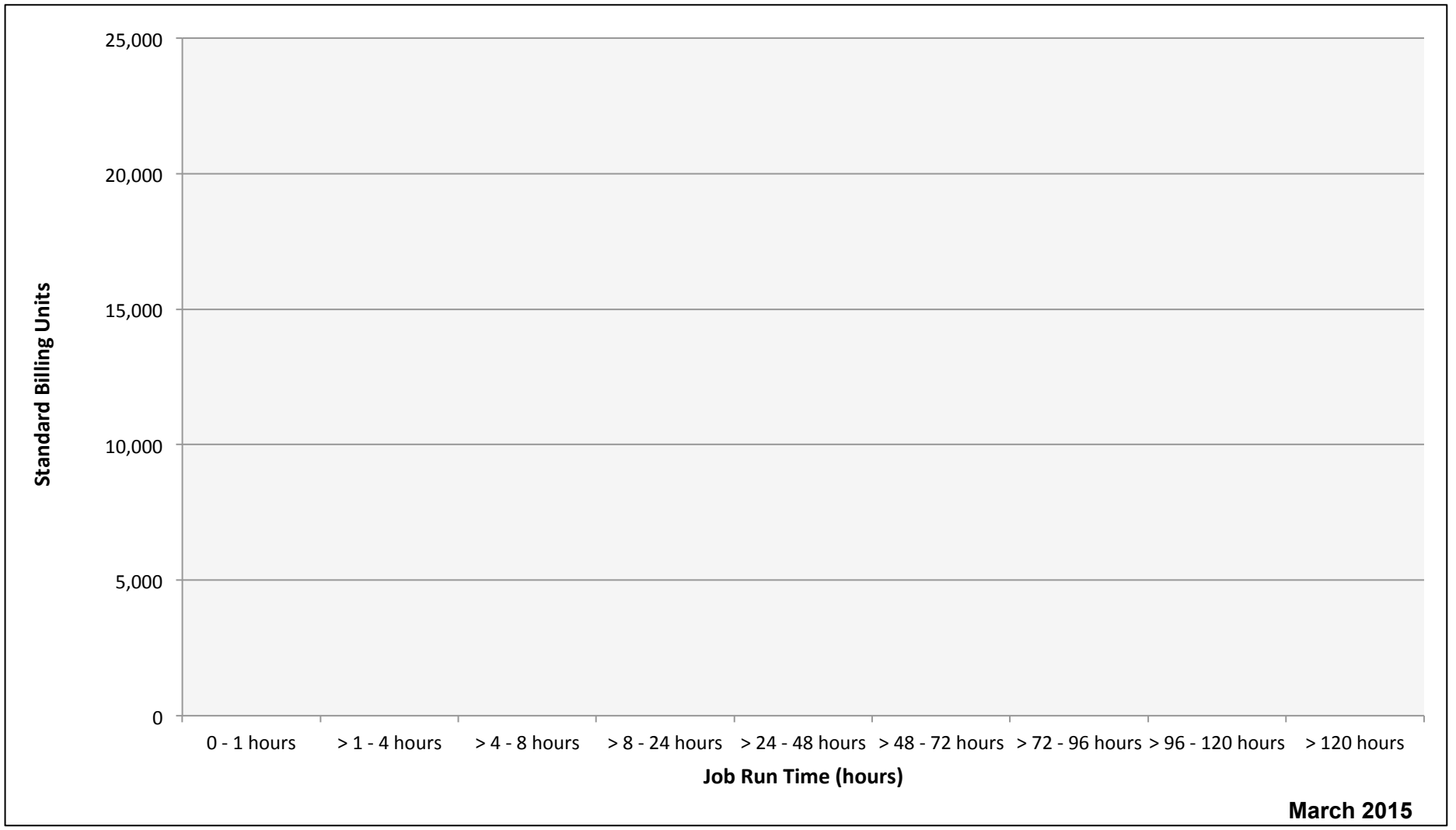
Endeavour:
Average Expansion Factor



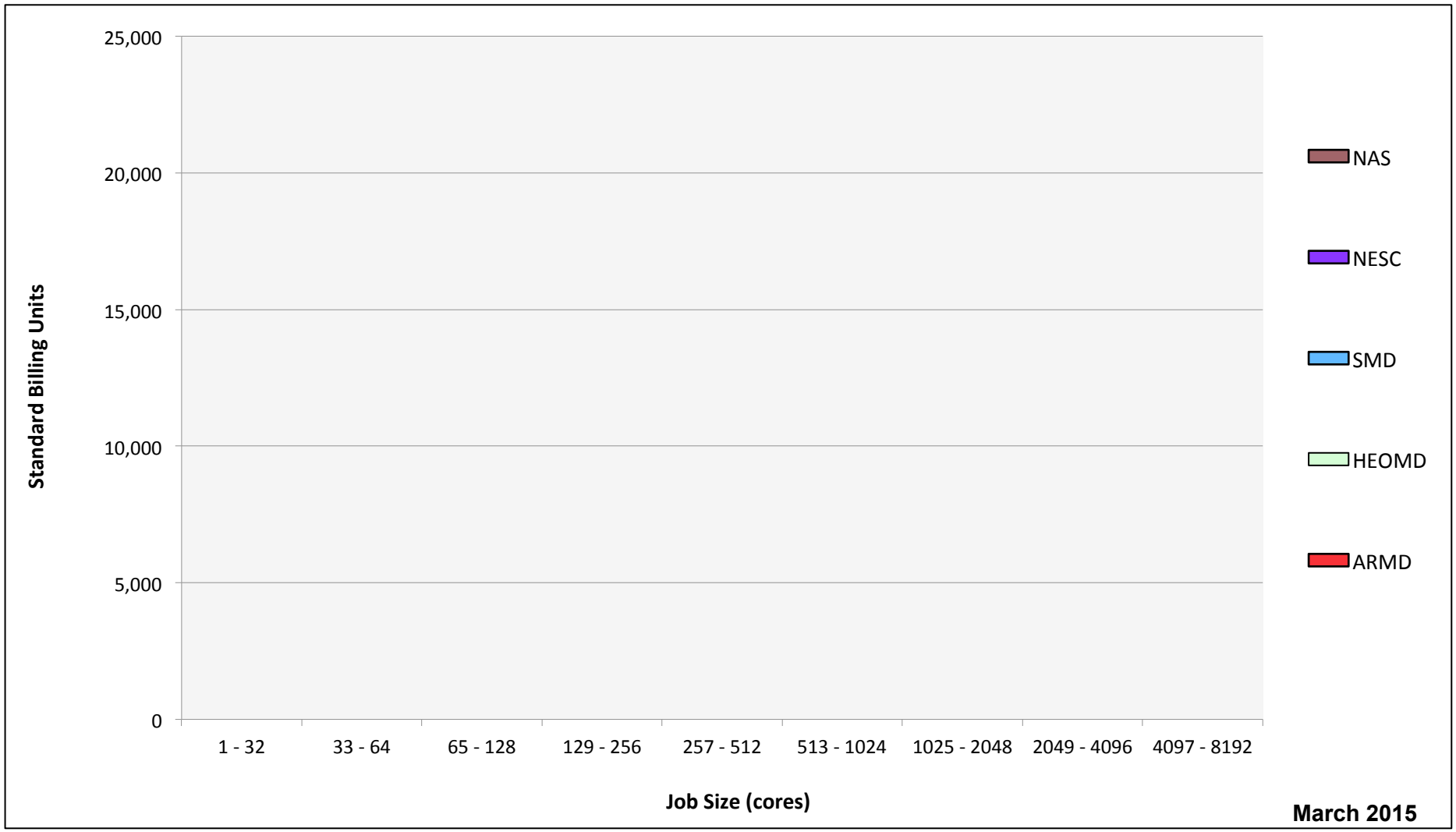
Merope:
SBUs Reported, Normalized to 30-Day Month



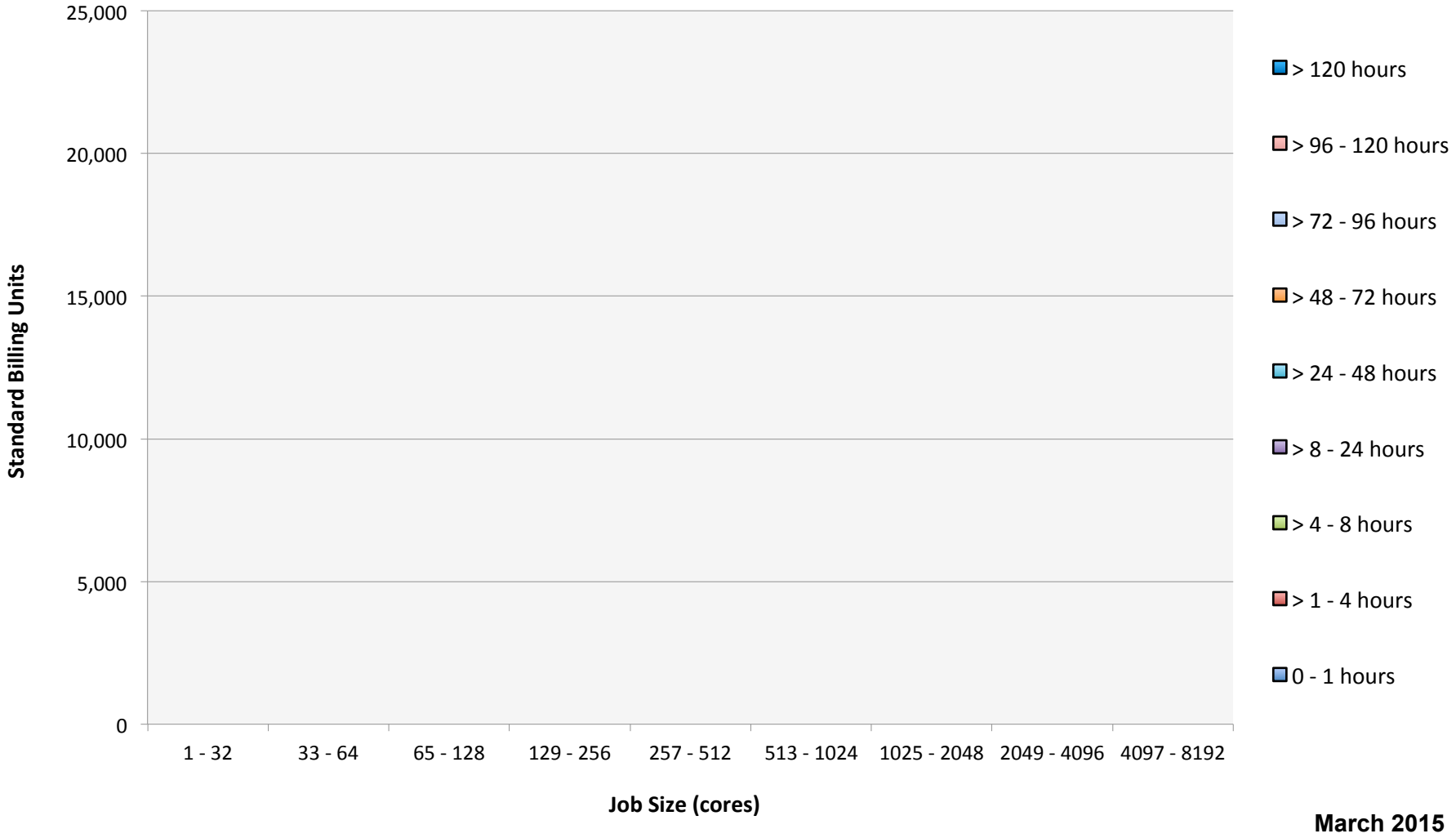
Merope:
Monthly Utilization by Job Length



Merope:
Monthly Utilization by Size and Mission



Merope:
Monthly Utilization by Size and Length



Merope:
Average Expansion Factor